**checkCIF/PLATON report**

Structure factors have been supplied for datablock(s) 1013\_0m\_a

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

[No syntax errors found. CIF dictionary Interpreting this report](http://journals.iucr.org/services/cif/checking/checkcifreport.html)

**Datablock: 1013\_0m\_a**

Bond precision: C-C = 0.0084 A Wavelength=0.71073

|  |  |  |  |
| --- | --- | --- | --- |
| Cell: | a=10.786(13) | b=12.175(10) | c=12.759(12) |
|  | alpha=69.30(3) | beta=89.17(5) | gamma=75.64(4) |
| Temperature: | 293 K |  |  |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | Calculated |  |  | Reported |
| Volume | 1513(3) |  |  | 1514(3) |
| Space group | P -1 |  |  | P -1 |
| Hall group | -P 1 |  |  | -P 1 |
| Moiety formula | C32 H12 F13 | O4 | Sb | C32 H12 F13 O4 Sb |
| Sum formula | C32 H12 F13 | O4 | Sb | C32 H12 F13 O4 Sb |
| Mr | 829.18 |  |  | 829.17 |
| Dx,g cm-3 | 1.820 |  |  | 1.819 |
| Z | 2 |  |  | 2 |
| Mu (mm-1) | 1.030 |  |  | 1.030 |
| F000 | 808.0 |  |  | 808.0 |
| F000’ | 807.50 |  |  |  |
| h,k,lmax | 12,14,14 |  |  | 12,14,14 |
| Nref | 5034 |  |  | 4983 |
| Tmin,Tmax | 0.697,0.884 |  |  | 0.708,0.886 |
| Tmin’ | 0.683 |  |  |  |

Correction method= # Reported T Limits: Tmin=0.708 Tmax=0.886

AbsCorr = MULTI-SCAN

Data completeness= 0.990 Theta(max)= 24.490

R(reflections)= 0.0346( 4500) wR2(reflections)= 0.1021( 4983) S = 1.057 Npar= 452

The following ALERTS were generated. Each ALERT has the format

**test-name\_ALERT\_alert-type\_alert-level**.

Click on the hyperlinks for more details of the test.

**Alert level C**



[ABSTY02\_ALERT\_1\_C](http://journals.iucr.org/services/cif/checking/ABSTY_02.html) An \_exptl\_absorpt\_correction\_type has been given without a literature citation. This should be contained in the

\_exptl\_absorpt\_process\_details field. Absorption correction given as multi-scan

[THETM01\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/THETM_01.html) The value of sine(theta\_max)/wavelength is less than 0.590

Calculated sin(theta\_max)/wavelength = 0.5833

[PLAT094\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT094.html) Ratio of Maximum / Minimum Residual Density .... 3.71 Report [PLAT148\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT148.html) s.u. on the a - Axis is (Too) Large .... 0.013 Ang. [PLAT242\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT242.html) Low ’MainMol’ Ueq as Compared to Neighbors of C4 Check [PLAT334\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT334.html) Small Aver. Benzene C-C Dist C1 -C6 1.37 Ang. [PLAT334\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT334.html) Small Aver. Benzene C-C Dist C41 -C46 1.37 Ang. [PLAT342\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT342.html) Low Bond Precision on C-C Bonds ............... 0.00841 Ang. [PLAT910\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT910.html) Missing # of FCF Reflection(s) Below Theta(Min). 8 Note [PLAT911\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT911.html) Missing FCF Refl Between Thmin & STh/L= 0.583 45 Report [PLAT971\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT971.html) Check Calcd Resid. Dens. 1.25A From C24 1.66 eA-3

[PLAT971\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT971.html) Check Calcd Resid. Dens. 1.41A From O2 1.60 eA-3

**Alert level G**



[PLAT012\_ALERT\_1\_G](http://journals.iucr.org/services/cif/checking/PLAT012.html) No \_shelx\_res\_checksum Found in CIF ...... Please Check [PLAT199\_ALERT\_1\_G](http://journals.iucr.org/services/cif/checking/PLAT199.html) Reported \_cell\_measurement\_temperature ..... (K) 293 Check [PLAT200\_ALERT\_1\_G](http://journals.iucr.org/services/cif/checking/PLAT200.html) Reported \_diffrn\_ambient\_temperature ..... (K) 293 Check [PLAT434\_ALERT\_2\_G](http://journals.iucr.org/services/cif/checking/PLAT434.html) Short Inter HL..HL Contact F6 ..F12 2.78 Ang.

1+x,y,-1+z = 1\_654 Check

[PLAT434\_ALERT\_2\_G](http://journals.iucr.org/services/cif/checking/PLAT434.html) Short Inter HL..HL Contact F7 ..F10 2.80 Ang.

1-x,2-y,1-z = 2\_676 Check

[PLAT710\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT710.html) Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 11 Do !

O1 -SB1 -O3 -C47 -116.00 2.00 1.555 1.555 1.555 1.555

[PLAT710\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT710.html) Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 28 Do !

O3 -SB1 -O1 -C37 -125.00 2.00 1.555 1.555 1.555 1.555

[PLAT909\_ALERT\_3\_G](http://journals.iucr.org/services/cif/checking/PLAT909.html) Percentage of I>2sig(I) Data at Theta(Max) Still 83% Note [PLAT933\_ALERT\_2\_G](http://journals.iucr.org/services/cif/checking/PLAT933.html) Number of OMIT Records in Embedded .res File ... 3 Note [PLAT978\_ALERT\_2\_G](http://journals.iucr.org/services/cif/checking/PLAT978.html) Number C-C Bonds with Positive Residual Density. 3 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

12 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

10 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

10 ALERT type 2 Indicator that the structure model may be wrong or deficient

6 ALERT type 3 Indicator that the structure quality may be low

2 ALERT type 4 Improvement, methodology, query or suggestion

0 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more

serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special\_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important

in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

**Publication of your CIF in IUCr journals**

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*[, you should make sure that full publication checks](http://journals.iucr.org/services/cif/checking/checkform.html) are run on the final version of your CIF prior to submission.

**Publication of your CIF in other journals**

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to

CIF submission.

**PLATON version of 07/08/2019; check.def file version of 30/07/2019**

**Datablock 1013\_0m\_a- ellipsoid plot**

>­

tD

lf)

tD

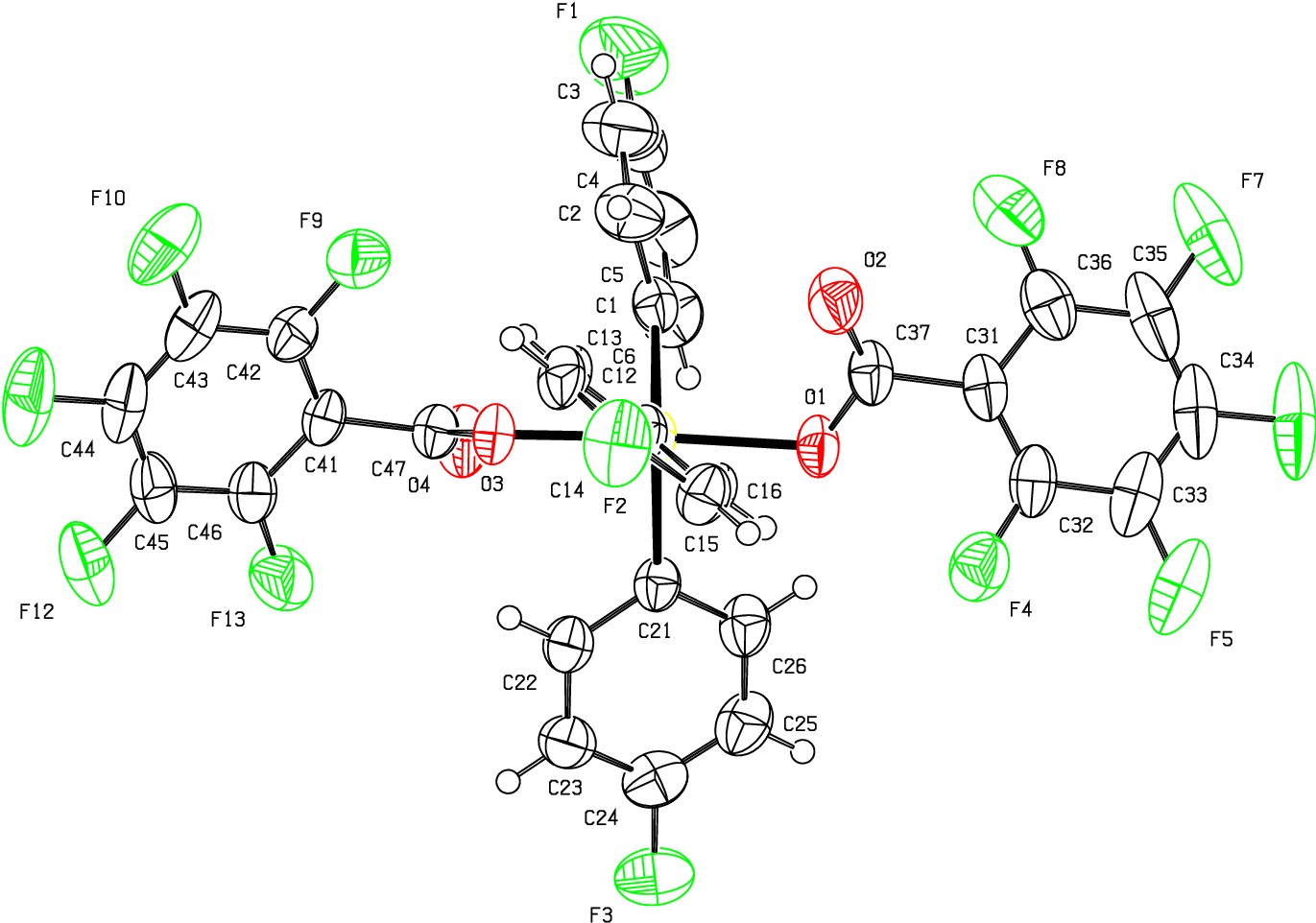
(Y")

0

r-

NOMOVE FORCED Prob

Temp



50

293

F6

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lf.).

CD

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f­

a:

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o\_

z 20

1013\_0m\_a P -1

R = 0.03 RES= 0

-55 X